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Topological susceptibility near T_c in SU(3) gauge theory

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ABSTRACT

Topological charge susceptibility χ_t for pure gauge SU(3) theory at finite temperature is studied using anisotropic lattices. The over-improved stout-link smoothing method is utilized to calculate the topological charge. Near the phase transition point we find a rapid declining behavior for χ_t with values decreasing from $(188(1)\ \text{MeV})^4$ to $(67(3)\ \text{MeV})^4$ as the temperature increased from zero temperature to $1.9T_c$ which demonstrates the existence of topological excitations far above T_c. The 4th order cumulant c_4 of topological charge, as well as the ratio c_4/χ_t is also investigated. Results of c_4 show step-like behavior near T_c while the ratio at high temperature agrees with the value as predicted by the diluted instanton gas model.

1. Introduction

Quantum Chromodynamics (QCD) is the gauge field theory that describes the rules of strong interaction among quarks and gluons, which has achieved great success in describing modern particle experiments. Higgs boson – used to be the last missing particle in this framework – was found in 2012 on LHC, claiming the landmark completeness of the Standard Model. From 2000s, lattice QCD which simulates QCD on finite lattices by powerful computers has gained enormous amount of results in accordance with experiments on accelerators, thanking for the incredible development of computers as well as the continuous progress in computational methods. Despite the success in the spectroscopy of hadrons, lattice QCD researchers have made great efforts on QCD thermodynamics with nonzero temperature and chemical potential, from which further understanding about hadronic matters and quark–gluon plasma can be obtained and problems such as the physics in early universe with extremely high temperature and density can be addressed.

Topology in lattice QCD has been widely studied for various purposes, while one of the most exciting applications is to explore the structure of QCD vacuum, which has not been well understood. The topological susceptibility χ_t has attracted special interest since 1979, when the quenched χ_t was related to the U(1) axial anomaly and mass of η' meson through the well-known Witten–Vaneziano relation [1,2]. Furthermore, the distribution of the topological charge Q can be described in terms of its cumulants [3]:

$$c_{2n} = \left.\frac{d^{2n} e_{vac}(\theta)}{d\theta^{2n}}\right|_{\theta=0}, \tag{1}$$

$$c_2 = \chi_t = \left.\frac{\langle Q^2\rangle}{V}\right|_{\theta=0}, \tag{2}$$

$$c_{2n} = (-1)^{n+1}\left[\frac{\langle Q^{2n}\rangle}{V} + \sum_{m=1}^{n-1}(-1)^m \binom{2n-1}{2m-1}\left\langle Q^{2(n-m)}\right\rangle c_{2m}\right], \quad n \geq 2 \tag{3}$$

where $e_{vac}(\theta)$ is vacuum energy density in the θ vacuum. The 2nd order cumulant c_2 is known as the topological susceptibility χ_t, and c_4 – the 4th order cumulant of Q is important to lattice calculations of observables with fixed topology sector [4,5]. Nonzero values for c_{2n} with $n > 1$ indicate non-Gaussian distri-

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bution of Q [6,7]. From (2) and (3), it is easy to see that $c_4 = -\left(\langle Q^4\rangle - 3\langle Q^2\rangle^2\right)/V$.

On the other hand, lattice studies of QCD at finite temperature and the phase structure of QCD have made great progress recently [8]. In particular, the relation between chiral symmetry breaking and deconfinement transition, as both of them happen to be near T_c, is of great importance and has attracted many researchers. Since χ_t describes the topological fluctuations of the vacuum in quenched situation, the behavior of χ_t near T_c is expected to provide a further understanding of the relation between chiral symmetry breaking and confinement.

Topological susceptibility at zero temperature for SU(3) gauge theory has been determined as $(191(5)\ \mathrm{MeV})^4$ [9]. χ_t at finite temperature also attracts great interest, especially around the transition temperature T_c [10–13]. In 2002, Gattringer et al. [12] found the cross-over behavior of χ_t in the temperature interval of $0.8T_c \sim 1.3T_c$, which is in accordance with results of other researchers. In their work chirally improved fermion action and fermionic method based on Atiyah–Singer index theorem were employed to calculate the topological charge. There are basically two kinds of methods to extract the topological charge: fermionic and bosonic method. For bosonic method, some kind of smoothing procedure is always to be applied first to dampen the fluctuations at the UV scale, while hopefully leaving the long range physics unchanged. In 2010 Lüscher proposed the Wilson flow method [14] that could be employed to calculate topological charge, which is renormalizable and converges to the continuum definition. More recently, Claudio Bonati et al. studied the dependence of 4D SU(N) gauge theories on the topological term at finite temperature by using cooling method [15], found that the θ dependence is drastically changed across the deconfinement transition. Moreover, the comparison between standard cooling method and Wilson flow method was also studied in Ref. [16], which led to equivalent results, both for average quantities and configuration by configuration. In this paper we present our work using over-improved stout-link smearing method [17] on the anisotropic lattices with a wider range of temperature to provide an alternative study on this interesting subject. This smearing method is based on the classical instanton solution in continuum limit, which is model dependent. However, it is observed that the method keeps the topological charge stable and always keeps values around the same integer obtained by the fermionic method. This method is also relatively cheaper than the other smoothing method. More recent studies were also carried out in Refs. [18–20] and part of their results are compatible with ours.

The diluted instanton gas model gives the ratio of c_4 and c_2 as the value -1 [21]. Recent calculation at zero temperature gives the ratio $R = -0.233(45)$ [7] (different definition of R leads to the opposite sign with ours in that paper), which is in contradiction with the value predicted by the diluted instanton gas model. At high temperature phase ($>1.15T_c$) the domination of the diluted instanton gas model was confirmed through the calculation of b_2 and free energy [15], where $b_2 = c_4/12\chi_t$. In this paper, we calculate the ratio $R = c_4/\chi_t$ below and above T_c with pure gauge configurations, trying to investigate the behavior of R around T_c using gluonic method.

This paper is organized as follows: we first present our lattice setup and details about extracting the topological charge Q at finite temperature. We also discuss the over-improved stout-link method to smooth the gauge field and the calculation of Q by field theoretical definition employing highly improved field strength tensor [22]. After that, results of Q and the susceptibility χ_t, as well as the 4th order cumulant c_4 of topological charge and the ratio R are presented and discussed. Finally main results of this paper are summarized.

2. Lattice setting and method

The calculation is carried out using anisotropic lattices, which have advantages of improving accuracy in lattice QCD for both zero and finite temperatures [23]. The Symanzik and tadpole improvement schemes of the gauge action are found to have better continuum extrapolation behaviors for many physical quantities, that is, the finite lattice spacing effect is well suppressed by these improvements. Considering these facts, we use the following improved gauge action, [24–26]

$$S_{IA} = \beta\left\{\frac{5}{3}\frac{\Omega_{sp}}{\xi u_s^4} + \frac{4}{3}\frac{\xi\Omega_{tp}}{u_t^2 u_s^2} - \frac{1}{12}\frac{\Omega_{sr}}{\xi u_s^6} - \frac{1}{12}\frac{\xi\Omega_{str}}{u_s^4 u_t^2}\right\} \tag{4}$$

where β is related to the bare QCD coupling constant g_0, $\xi = a_s/a_t$ is the aspect ratio for anisotropy (we take $\xi = 5$ in this work), u_s and u_t are the tadpole improvement parameters of spatial and temporal gauge links respectively. $\Omega_C = \sum_C \frac{1}{3}\mathrm{ReTr}(1 - W_C)$, with W_C referring to the path ordered product of link variables along a closed contour C on the lattice. Ω_{sp} includes the sum over all spatial plaquettes on the lattice, Ω_{tp} includes the temporal plaquettes, Ω_{sr} includes the product of link variables about planar 2×1 spatial rectangular loops, and Ω_{str} refers to the short temporal rectangles (one temporal link, two spatial). Practically, u_t is set to 1, and u_s is defined by the expectation value of the spatial plaquette $P_{ss'}$: $u_s = \left\langle \frac{1}{3}\mathrm{Tr}P_{ss'}\right\rangle^{1/4}$. Besides, it has been shown in Ref. [27] that the renormalization effects of the anisotropy ξ is ignorable as β varies. We also have used Wilson flow method to calculate the renormalized anisotropy according to Ref. [28] at different temperature with $\beta = 3.2$, and the results show that the differences between the renormalized ξ and bare ones are always less than 2%. We adopt anisotropic lattices with smaller a_t compared to a_s, so that we can investigate higher temperature with small spatial lattice size.

2.1. The definition of temperature

The temperature on lattice is defined as follow:

$$T = \frac{1}{N_t a_t}, \tag{5}$$

where N_t is the temporal lattice size. T can be changed by varying either N_t or the coupling constant β, which is related directly to the lattice spacing a_t. The critical temperature is determined for a given lattice $N_t = 24$ after the critical coupling β_c has been determined. The order parameter for determining β_c is chosen to be the susceptibility χ_P of the Polyakov line, which is defined as

$$\chi_P = \langle\Theta^2\rangle - \langle\Theta\rangle^2, \tag{6}$$

where Θ is the Z_3 rotated Polyakov line defined via:

$$\Theta = \begin{cases} \mathrm{Re}P\exp[-2\pi i/3] & \arg P \in [\pi/3, \pi) \\ \mathrm{Re}P & \arg P \in [-\pi/3, \pi/3) \\ \mathrm{Re}P\exp[2\pi i/3] & \arg P \in [-\pi, -\pi/3) \end{cases} \tag{7}$$

and P represents the trace of the spatially averaged Polyakov line for each gauge configuration. After a rough scan, a more refined study for the peak position of the susceptibility χ_P gives the critical coupling constant $\beta_c = 2.808$, which corresponds to the critical temperature $T_c \approx 0.724 r_0^{-1} = 296$ MeV [27]. Here r_0 is the hadronic scale parameter and we take $r_0^{-1} = 410\,(20)$ MeV.

Considering both finite volume effects and good resolution of temporal lattice at $T \sim 2T_c$, we set $\beta = 3.2$ in the study of topological susceptibility at finite temperature. The corresponding lattice spacing a_s is obtained by calculating the static quark potential

$V(r)$ on an anisotropic lattice $24^3 \times 128$. The fitting result of string tension σ reads:

$$\frac{a_s}{r_0} = \sqrt{\frac{\sigma a_s^2}{1.6 + e_c}} = 0.1825\,(7)\,, \tag{8}$$

taking $r_0^{-1} = 410\,(20)$ MeV, we have $a_s = 0.0878\,(4)$ fm. Comparing to a_s at $\beta_c = 2.808$ and $N_t = 24$, the approximate values for N_t that corresponding to T_c and $2T_c$ at fixed $\beta = 3.2$ can be calculated and the results are $N_t \sim 38$ and $N_t \sim 19$ respectively. More parameter details can be found in Ref. [23]. It should be pointed out that the difference between T_c ($\beta = 2.808$) and T_c ($\beta = 3.2$) is negligible due to the application of the improved gauge action.

In this study we change the temperature by varying temporal lattice size N_t. Working on the same β which corresponding to the same a_s makes all our lattices share the same spatial volume while the temperature T varies in a wide range. This avoids the influence from possible finite volume effects arising from different spatial volumes. Setting $\beta = 3.2$, we generated a series of lattice $24^3 \times N_t$ with $N_t = 20, 24, 28, 32, 36, 40, 44, 48, 60, 80$ and 128, which cover the range of $T \in [0.3T_c,\ 1.9T_c]$, and the spatial size $L_s \approx 2.1$ fm. For each anisotropic lattice with a fixed value of N_t, we sampled roughly 1000 configurations (1900 for $N_t = 60$), after 10 000 sweeps from cold start and with 500 sweeps between each sampling. Here one sweep consists of a composite update of 1 pseudo heat-bath and 5 over-relaxation procedures over all link variables. 5000 samples of 24^4 isotropic lattice with the same a_s were also generated and measured as the results at zero temperature. We roughly estimated the integrated autocorrelation time of topological charge τ_Q, which is about 200 sweeps at zero temperature and about 440 sweeps at $1.9T_c$.

2.2. Over-improved stout-link method

It is well-known that the topological charge Q calculated directly from a typical lattice configuration by the field theoretic definition [29,30]:

$$Q = \frac{1}{32\pi^2}\int d^4x\, \mathrm{tr}\left(F_{\mu\nu}\tilde{F}_{\mu\nu}\right), \tag{9}$$

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig\left[A_\mu, A_\nu\right], \quad \tilde{F}_{\mu\nu} = \frac{1}{2}\epsilon_{\mu\nu\rho\sigma}F_{\rho\sigma}, \tag{10}$$

will not be an integer in general, which is obviously conflicting with the continuum situation. Thus, some cooling or smearing procedure is essentially to be taken on original configurations before calculating Q by bosonic methods, aiming to suppress the ultraviolet fluctuations. Highly improved lattice field-strength tensor [22] is also helpful to obtain an integer Q on the lattice, as we used 1×1, 2×2 and 3×3 3-loop improved $F_{\mu\nu}$ which is practically good enough.

All cooling or smearing methods are based on an approximation to the continuum gauge field action:

$$S_g = \frac{1}{2}\int d^4x\, \mathrm{tr}\left[F_{\mu\nu}F_{\mu\nu}\right], \tag{11}$$

and the lattice version of S_g contains combination of plaquette and larger Wilson loops. However, the discretization error always exists, which is harmful to the topological objects and smoothing procedure. So in these methods the destruction of topological structure is unavoidable. For the purpose of the study on topology susceptibility, we adopt the over-improved stout-link smearing method developed by Moran and Leinweber [17] to filter the lattice, which is proved to be efficient in preserving instanton-like objects.

Over-improved stout-link smearing method introduces the over-improved parameter ϵ [31] into stout-link smearing algorithm [24]. The improved action with instanton solution substituted reads:

$$S^{inst}(\epsilon) = \frac{8\pi^2}{g^2}\left[1 - \frac{\epsilon}{5}\left(\frac{a}{\rho_{inst}}\right)^2 + \frac{14\epsilon - 17}{210}\left(\frac{a}{\rho_{inst}}\right)^4\right], \tag{12}$$

where ρ_{inst} is the instanton size. Negative ϵ leads to a positive leading order error term of ρ_{inst}^{-2}, which means instanton-like objects will be preserved when the action is reduced in smoothing procedure. The modified link combination used by over-improved stout-link method is as follow:

$$\begin{aligned} \mathcal{C}_\mu(x) = \rho_{\rm sm}\sum\bigg\{ & \frac{5-2\epsilon}{3}\left(1\times1 \text{ paths touching } U_\mu(x)\right) \\ & - \frac{1-\epsilon}{12}\left(1\times2 + 2\times1 \text{ paths touching } U_\mu(x)\right)\bigg\}. \end{aligned} \tag{13}$$

There are three free parameters in the over-improved stout-link smearing method: the over-improved parameter ϵ, the smearing parameter $\rho_{\rm sm}$, and $n_{\rm sm}$ – the number of smoothing steps taken on each configuration. Moran and Leinweber had practically determined $\epsilon = -0.25$ to maximize the life of instantons under iterative smearing procedure, which we also kept fixed in our study. We check this on several configurations at different temperature and confirmed that topological charge approaches integral number quickly as long as $n_{\rm sm} \geq 10 \sim 40$ in most situation, and keeps almost the same value for thousands of steps, which will be presented at the last of this sector.

For the other two parameters $\rho_{\rm sm}$ and $n_{\rm sm}$, we perform some tests to find suitable values for them. Five configurations are investigated for each temperature and smoothed 200 times for $\rho_{\rm sm} = 0.01 \sim 0.08$, and the results of topological charge for some typical values of $\rho_{\rm sm}$ are shown in Fig. 1. It's obvious that the larger $\rho_{\rm sm}$ becomes, the faster the topological charge becomes an integer. However, in practice we found that when $\rho_{\rm sm}$ is equal to or larger than about 0.08, smoothing leads to completely unstable results, as shown in lower right panel in Fig. 1, which is the same situation for all N_t. Finally we set $n_{\rm sm} = 40$ and $\rho_{\rm sm} = 0.05$ for all lattices (except for $N_t = 128$ we set $\rho_{\rm sm} = 0.07$, keeping $n_{\rm sm} = 40$).

By the way, we check the stability of the over-improved stout-link smearing method, which is supposed to be an effective and cheaper method (compared to the fermionic method) to suppressing the ultraviolet fluctuations on the lattices while preserving topological structures as long-lived as possible during smoothing. One of the most important problems of smoothing-type methods is the instability of topological charge when smoothing is carried out. We made several tests to check this, such as 10 000 steps smearing on different configurations with nonzero topological charge Q both below and above T_c. Part of the results are shown in Fig. 2. It indicates that, within the over-improved stout-link smearing method, with proper parameters and improved field strength tensor adopted, one can preserved instanton-like objects for long enough time without causing the system to fall into the trivial topological sector. Therefore, the result for the topological charge is robust and almost independent of the number of smoothing steps once an integral value for Q is obtained for most of configurations. Notice that we measure the topological charge after every 500 steps of smoothing in stability tests while for most of configurations Q is almost an integer after about 40 steps.

3. Results and discussion

We extract 1000 topological charge data for each temperature on anisotropic lattices and 5000 samples on 24^4 isotropic lattice,

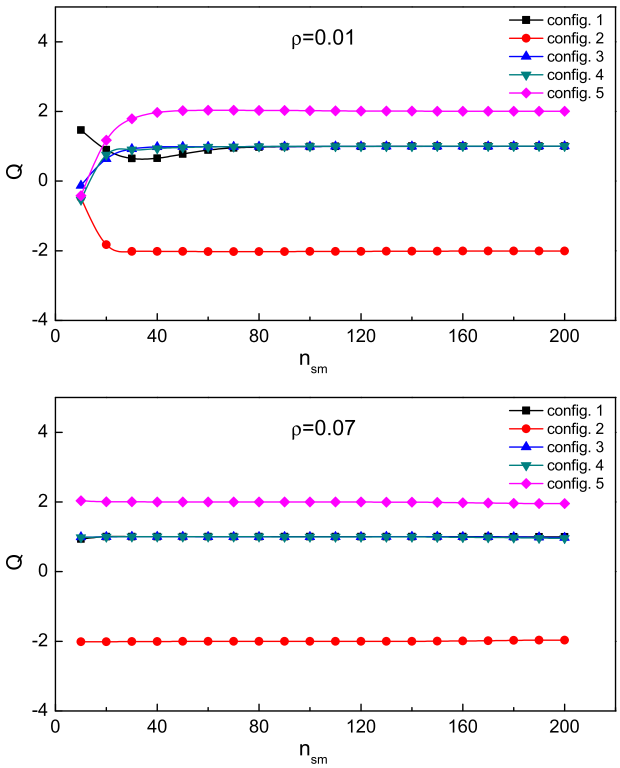

Fig. 1. Smooth tests for different ρ at $N_t = 40$. Tests at other temperatures show similar situation, except that at lower temperatures, more steps are needed to extract the nearly integer values of Q.

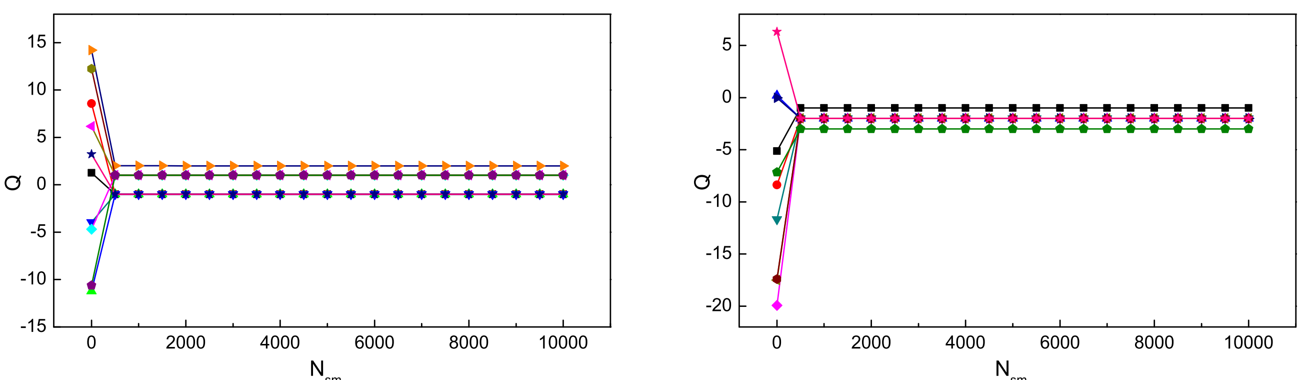

Fig. 2. Stability tests at $T = 1.19T_c$ (left) and $T = 0.79T_c$ (right) on 10 configurations with nonzero Q.

which are all obtained after 40 steps of smoothing procedures. Most of these values are nearly integers. Those Q values that deviate larger than 0.1 from an integer – which we called "bad points" – are less than 4% for each lattice setting. The number of "bad points" grows slightly as the temperature approaches zero and for $N_t = 128$ (corresponding to nearly zero temperature) we set $\rho_{\rm sm} = 0.07$ to ensure that 40 steps of smooth are practically enough to avoid too much "bad points".

Firstly, we display the histograms of the topological charge Q for different temperatures in Fig. 3. As the temperature increases, distribution of Q becomes narrower as expected, that the topological excitations are suppressed above T_c. We fit the histograms of Q with a Gaussian function which are denoted as the blue lines in Fig. 3. The deviation from the Gaussian distribution comes from nonzero higher order cumulants and limited sampling.

Next, the susceptibility χ_t and the 4th-order cumulant c_4 of Q as well as the ratio R are worked out at different temperatures, and the results are shown in Fig. 4, Fig. 5 and Table 1 where the errors are statistical and estimated by jackknife method. These quantities from original topological charge data as well as Q after rounding off are calculated, which make almost no differences. So the presented results are based on original Q measured.

The susceptibility at $T = 0$ reads $\chi_t = (188(1)\ \text{MeV})^4$ which is consistent with former results by other methods. It also clearly shows that topological excitation exists even at $T = 1.9T_c$, where $\chi_t = (67\ \text{MeV})^4$ and 4.2% configurations have nonzero topological charge. That means instanton-like structures may exist even above T_c to nearly $2T_c$ supporting the conclusion of Gattringer et al. As Fig. 4 shows, a crossover behavior for χ_t decreasing from $(188(1)\ \text{MeV})^4$ to $(67(3)\ \text{MeV})^4$ is found. For all configurations below T_c (from 0 to $0.95T_c$), χ_t stays around $(177\ \text{MeV})^4 \sim (189\ \text{MeV})^4$. From $24^3 \times 36$ configurations corresponding to $1.05T_c$, χ_t starts to decline as the temperature increases. Notice that Fig. 4 shows the value of $\chi_t^{1/4}$, and χ_t decreases much faster than seen above T_c, consistent with results in Ref. [12]. For example, at $T = 1.05T_c$ where $\chi_t = (148\ \text{MeV})^4$

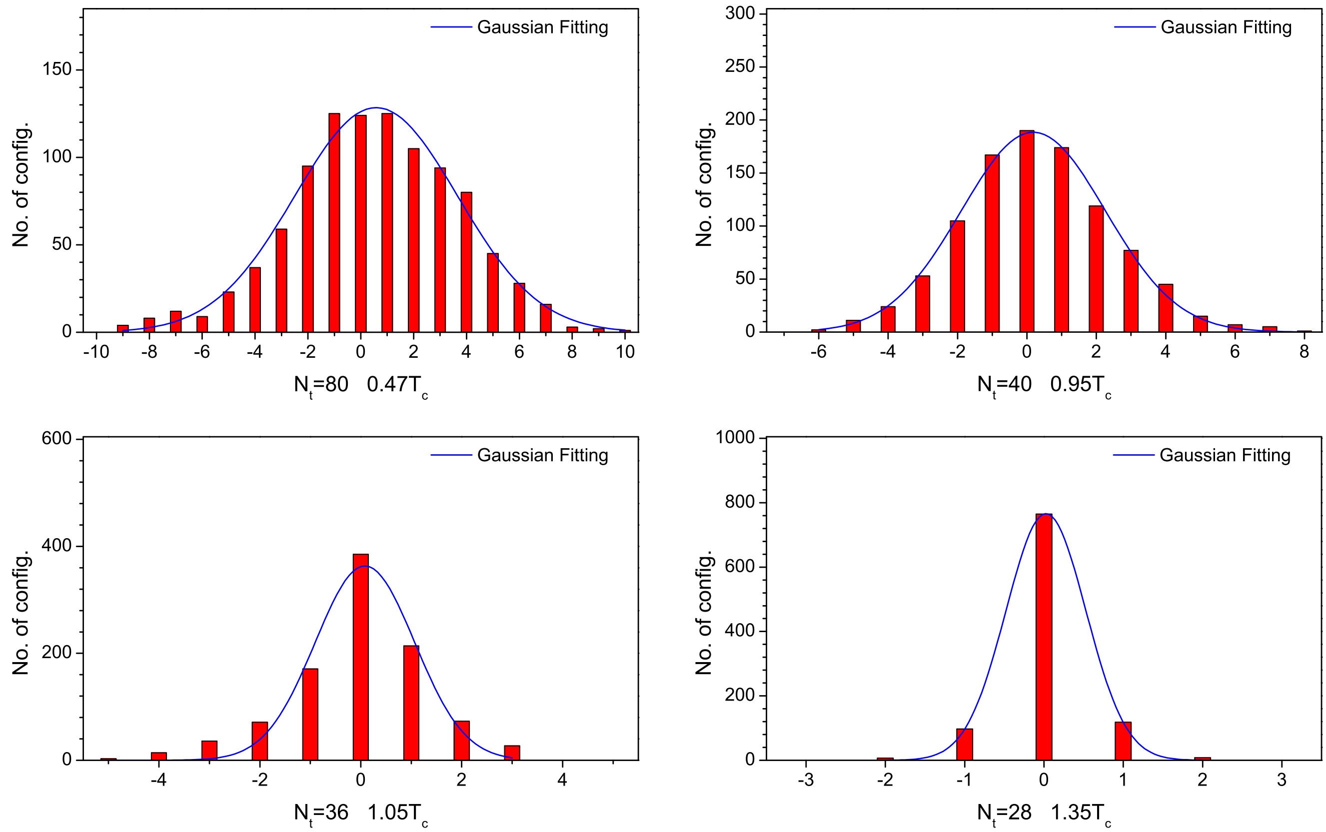

Fig. 3. Distribution of the topological charge at different temperature.

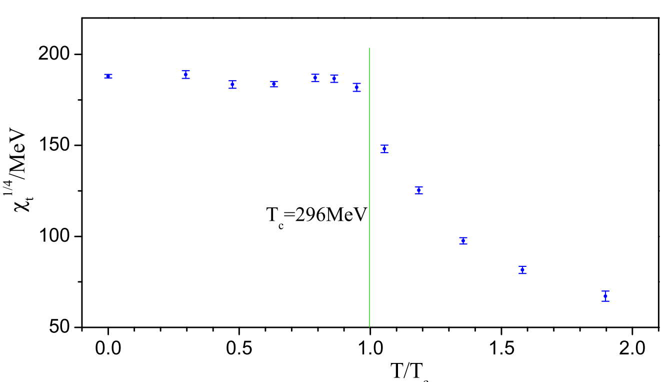

Fig. 4. Results for $\chi_t^{1/4}$ vs. temperature.

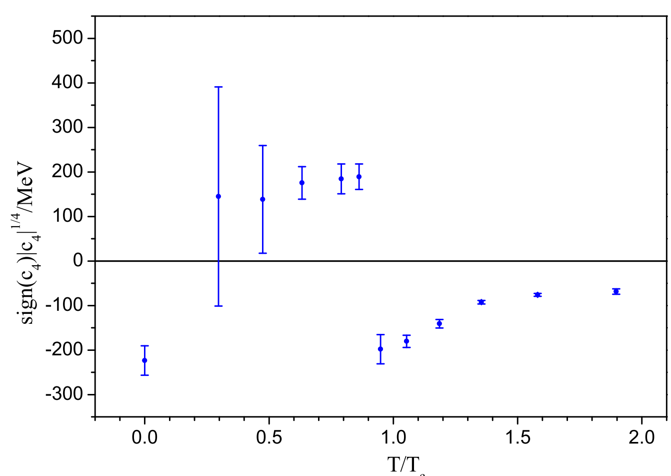

Fig. 5. $c_4^{1/4}$ of Q. For convenient, we show $|c_4|^{1/4}$ with the same sign of c_4.

which is 38.4% of its zero-temperature value, while at $T = 1.9T_c$, $\chi_t = (67\text{ MeV})^4$ has dropped to about only 1.6% of its zero-temperature value. The value of χ_t remains almost constant below T_c and declines rather rapidly from $0.95T_c$ to $1.05T_c$ signaling for the phase transition.

As shown in Table 1, R approaches -1 from below in the interval $[1.05T_c, 1.19T_c]$ as T grows, while above $1.35T_c$ R values not far away from -1, in agreement with the result of Ref. [32], in which $b_2 = R/12$ approaches $-1/12$ from below as T goes beyond $1.15T_c$ or so. This is also consistent with the value predicted by the diluted instanton gas model. Similar coincidence has also been found in a recent separate lattice study [33]. Besides, although the error bars grow larger as the temperature approaches zero, c_4 shows a step-like behavior near T_c that could be seen in Fig. 5. However, these behaviors couldn't be the proof of the existence of discontinuity between $0.86T_c$ and $0.95T_c$, that may be related to chiral and deconfinement phase transition, and should be carefully examined with more accurate calculations and finer temperature resolution. It is also found that, for pure gauge theories, the calculations of c_4 and R do need much more samples to suppress the static errors, so we can't make any conclusion from the results of c_4 and R near $T = 0$. The statistical errors of χ_t and c_4 could be evaluated according to [6], which indeed shows much noisier signals of c_4 than those of χ_t near zero temperature.

4. Summary

Topological susceptibility and the 4th order cumulant of topological charge in pure SU(3) gauge theory are calculated using

Table 1
$\chi_t^{1/4}$, c_4 and R at different temperatures. Last row is corresponding to isotropic configurations at $T = 0$.

Config.	T/MeV	T/T_c	$\chi_t^{1/4}$/MeV	c_4/MeV^4	$R(c_4/\chi)$
$24^3 \times 20$	562	1.90	67(3)	$-(69(6))^4$	−1.09(26)
$24^3 \times 24$	468	1.58	82(2)	$-(76(3))^4$	−0.75(10)
$24^3 \times 28$	401	1.35	98(2)	$-(93(4))^4$	−0.81(11)
$24^3 \times 32$	351	1.19	125(2)	$-(141(10))^4$	−1.58(36)
$24^3 \times 36$	312	1.05	148(2)	$-(180(14))^4$	−2.20(60)
$24^3 \times 40$	281	0.95	182(2)	$-(198(33))^4$	−1.38(84)
$24^3 \times 44$	255	0.86	187(2)	$(189(29))^4$	1.05(62)
$24^3 \times 48$	234	0.79	187(2)	$(184(33))^4$	0.94(68)
$24^3 \times 60$	187	0.63	184(1)	$(175(37))^4$	0.83(72)
$24^3 \times 80$	140	0.47	183(2)	$(138(121))^4$	0.31(1.16)
$24^3 \times 128$	88	0.30	189(2)	$(145(246))^4$	0.32(2.78)
$24^3 \times 24$	0	0	188(1)	$-(223(33))^4$	−2.00(1.14)

anisotropic lattices from zero temperature to $1.9T_c$. The computation utilizes over-improved stout-link smearing method, employing 3-loop highly improved field strength tensor. The results obtained are consistent with than existing results in literatures using other methods, while extended to higher temperature. Once appropriate parameters are adopted, it is confirmed that the value of the topological charge is stable and robust during the smoothing procedure after becoming an integer. We also confirm the existence of topological excitations around $1.9T_c$. The asymptotic behavior of the ratio c_4/χ_t above $1.19T_c$ is consistent with the diluted instanton gas model. Furthermore, a step-like behavior of c_4 around T_c inspires further investigation of high order cumulants of topological charge.

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